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Final Report

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Principal Investigator - Robert V. Edwards
Chemical Engineering Department
Case Western Reserve University
Cleveland, OH 44106

Maximum Likelihood Techniques Applied to Quasi-Elastic Light Scattering

By now, everyone involved with QEELS knows that any method for extracting particle size information must involve a methodology that contains mathematical assumptions brought to the problem by the experimenter. This comes about because the measurement technique itself obtains a very indirect measurement of a signal derived from the motion of the particles in the system.

Getting particle size information from the process requires the solution of an noisy "inverse problem." The noise in the system has two primary sources: the photon detection process itself, and the fact that the particle signal is a random variable. Unfortunately, the inverse problem so generated is notoriously difficult to solve. Dr. R. Pike has elegantly shown how the eigenvalue structure of the transform that generates the signal is such that an arbitrarily small amount of noise can obliterate parts of any practical inversion spectrum.

An additional problem, indeed the one that generated this project, is the necessity of coming up with an automatic procedure for reliable estimation of the quality of the measurement process. This was motivated by the desire to have a software supervisor system that was capable of operating unmanned, as might be needed in a space flight experiment. Statistical methodologies such as Maximum Entropy Parameter Estimation and Maximum Likelihood Estimation offered a framework that could provide such information.

We started a project to use Maximum Likelihood Estimation (MLE) as such a framework. The idea was to generate a theory and a functioning set of software to oversee the measurement process and extract the particle size information, while at the same time providing error estimates for those measurements. The error estimates could be used to assess the overall status of the measurement system and to set up the operating conditions for successful measurements.

Initially, I rewrote the basic theory for the QEELS method in order to clarify the role of the optics and the data processing system. Another important part of this report was estimation of the noise covariance matrix. Knowledge of this term is critical to evaluation of any measurement scheme. This report was delivered to NASA, in June 1989.

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Outline of the Theory

The key concept in any of the inversion methods is a quantity that can be defined as the probability of the measured data set, given a set of parameters for the model the data is being compared to.

Let $p(\{d_n\} | \alpha)$ be the probability described above. The data set is denoted $\{d_n\}$, and the set of parameters is given by the vector α . An approximate form for the log of this probability is given by

$$\ln(p(\{d_n\} | \alpha)) \approx \sum_n \sum_m (d_n - f(n, \alpha)) \Lambda_{nm}^{-1} (d_m - f(m, \alpha)),$$

where Λ_{nm} is the covariance matrix for the noise on the measurement, and $f()$ is the model function for the expected measurement as a function of the parameter set, α . Solution for the parameters means maximizing the log of the probability, or in the case of Maximum Entropy Estimation, maximizing a function of the log of the probability. It should be obvious that the form of the covariance is critical to a correct solution to the problem.

Further, error estimates for the measurements are obtained from the same function, viz.

$$\sigma_i^2 \approx \left\langle -\frac{\partial^2 \ln(p)}{\partial \alpha_i \partial \alpha_j} \right\rangle^{-1},$$

where $\langle \rangle$ denotes expected value of the expression contained within the brackets. The error estimates of the measured parameters is given by the diagonal elements of the inverse of the matrix of expected second derivatives of the probability with respect to the parameters. Again, the correct form for the covariance matrix is critical.

Our Work

In over 99% of the literature, the covariance matrix is either ignored or assumed to be a diagonal matrix. This certainly simplifies the mathematics necessary, but gives misleading results. In statistical language, assuming the matrix is diagonal vastly overestimates the number of degrees of freedom in the data. A non-diagonal covariance matrix will show up on a correlogram as hills and valleys whose extent is about the correlation length of the data.

Experimentalists in the field are becoming sensitive to the need for some kind of error estimate for their measurements, but rarely take the simple step of running multiple measurements of the same system to generate a measured error estimate to validate the theoretical ones derived from the oversimplified noise models. If they have done these checks, the literature is strangely silent on that fact.

We set out to verify a correct form for the covariance matrix and then use it to generate software to estimate particle size parameters using a modified histogram approach. This method was to be extended to multiple angle experiments, if possible.

The covariance matrix was to be measured directly by performing multiple (over a thousand) identical measurements of the same set of particles. Our existing autocorrelation computers were not reliable enough for such measurements, so we were in the process of building a new correlator with the required flexibility and stability to be able to do the measurements.

While I was waiting for the correlator to be completed, I set out to write some software using a diagonal covariance matrix in order to provide a convenient basis of comparison for the routines to be developed. I was doing the modeling in the APL programming language. Parallel to my efforts, I had a student writing code in C. His program was supposed to be structured so that it could be used with all the conceivable algorithms I anticipated in this project. That student did not do so well. The code was never completed.

When I got my code running, I was shocked at how sensitive the program was to small changes in the data. This was the direct result of the sensitivity of the algorithm to small changes in the probability function. A change of less than 0.01 % in the probability can result in a changes of over 100% in several of the parameters being estimated. Worse, there was no clue as to this problem in the literature.

As a result, I was forced to write my own maximization routines, based on so-called Davidon-Fletcher-Powell (DFP) procedures. My strength is not numerical programming, so it was a struggle to construct a successful program. I did succeed. I will argue that it is the best least squares, histogram extracting program for QELS. It is slow and its input-output is not elegant, but it does work. This software was supplied to NASA Lewis, but I have never heard how it performed on their data.

The third year of the project was with zero funding, so I was working alone.

The software was modified to work on multiple angle data. It worked poorly. After examining the data carefully, I was forced to conclude that the problem was that the covariance matrix is not diagonal. The hills and valleys on one data set do not correspond to the hills and valleys on different sets of data. Proper software for multiple angle experiments will have to await the results of the calculations for the covariance.

Synopsis

1. The framework for using MLE to supervise and analyze QELS experiments was written and delivered to NASA. Given time, this will be turned into a published paper in the near future.
2. The autocorrelation computer is completed and tested. It is ready for the experiments on the covariance.
3. Software for maximizing the probability functions has been created and delivered to NASA. In its present realization, it assumes a diagonal covariance matrix, however, it can easily be modified to handle more realistic situations. At Bill Meyers' urging, Dr. Bones sent me some code for efficient inversion of the covariance matrix.

We have neither received nor generated any classified material as a result of this project.